Analysis of Neutron Thermal Scattering Data Uncertainties in PWRs

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Outline

PART I. Random STLs

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I.4 Correlation Matrix for Inelastic Cross Section: H-H2O

I.5 Thermal Scattering Processed Data

I.6 Application to Criticality Benchmarks moderated by H2O

I.7 Analysis of the Importance of PDF

Ref. "*Random Adjustment of the H in H2O Neutron Thermal Scattering Data*",
D. Rochman and A. J. Koning, NUCLEAR SCIENCE AND ENGINEERING: **172**, 287–299 (2012)

I.1 Model for Thermal Neutron Scattering

In the case of H in H2O, incoherent inelastic scattering is the major component, and coherent and incoherent elastic scattering can be neglected. Inelastic scattering is described by the scattering law *S(*α,β), asymmetric form of the scattering law, at different temperatures:

The double-differential scattering cross section for thermal neutrons

$$\frac{\partial^2\sigma(E \to E',\mu)}{\partial E'\partial\mu} = \frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}S(\alpha,\beta)$$

the momentum transfer

$$\alpha = \frac{E + E' - 2\sqrt{EE'}\mu}{AkT}$$

the energy transfer

$$\beta = \frac{E' - E}{kT}$$

S(α,β) is the Fourier transform of the intermediate scattering function

$$S(\alpha,\beta) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{i\beta\hat{t}}e^{-\gamma(\hat{t})}\,d\hat{t}$$

γ(t), the intermediate scattering function

$$\gamma(\hat{t}) = \alpha\int_{-\infty}^{+\infty} P(\beta)(1 - e^{-i\beta\hat{t}})e^{-\beta/2}\,d\beta$$

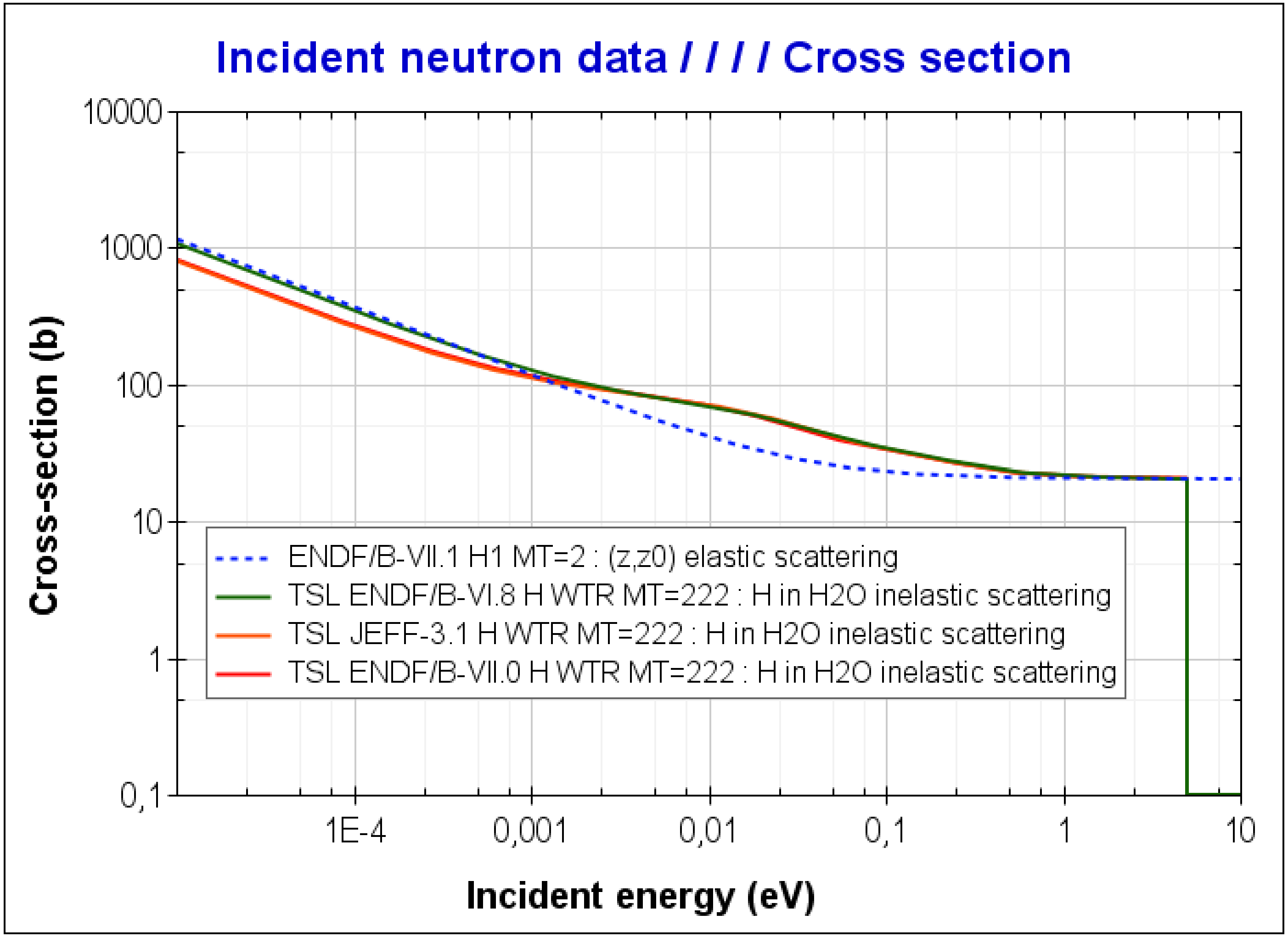
, where:

$$P(\beta) = \frac{\rho(\beta)}{2\beta\sinh(\beta/2)}$$

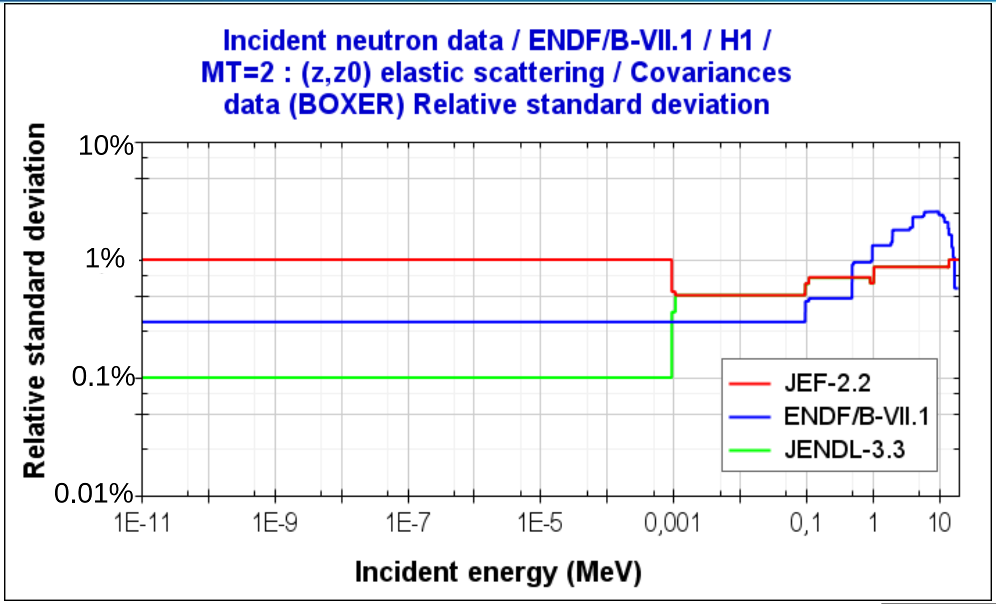
The frequency spectrum

$$\rho(\beta) = \sum_{i=1}^{K}\rho_i(\beta) \quad \begin{cases} \rho_i(\beta) = \omega_i\delta(\beta_i) \text{ for the discrete oscillators} \\ \rho_i(\beta) = \rho_s(\beta) \text{ for the solid-type spectrum} \\ \rho_i(\beta) = \rho_t(\beta) \text{ for the translational spectrum} \end{cases}$$

Comparison of Elastic Cross Section: H (free gas model) versus H-in-H2O

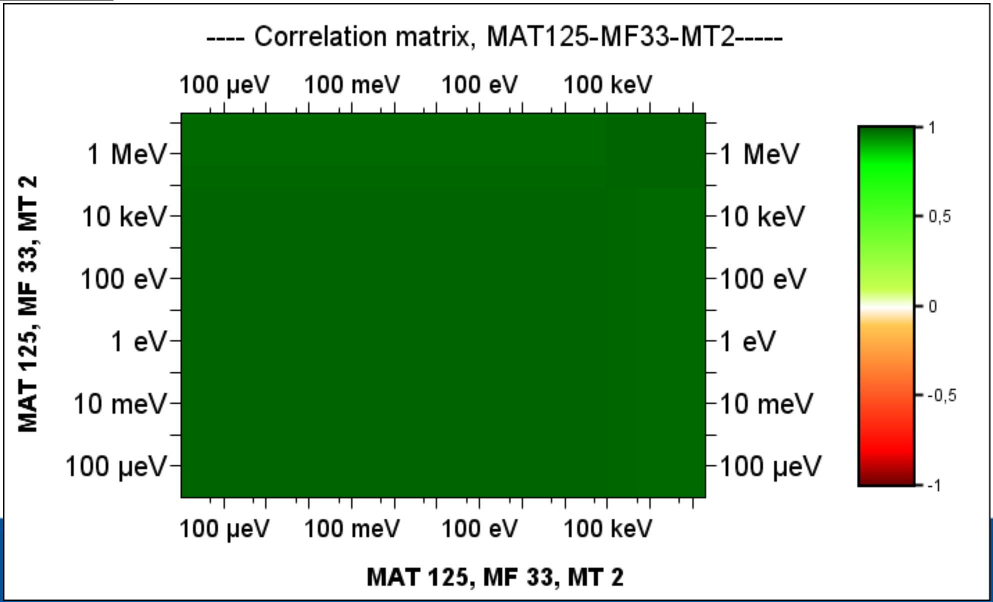


ENDF Uncertainties: Elastic Cross Section (MT2) for Hydrogen

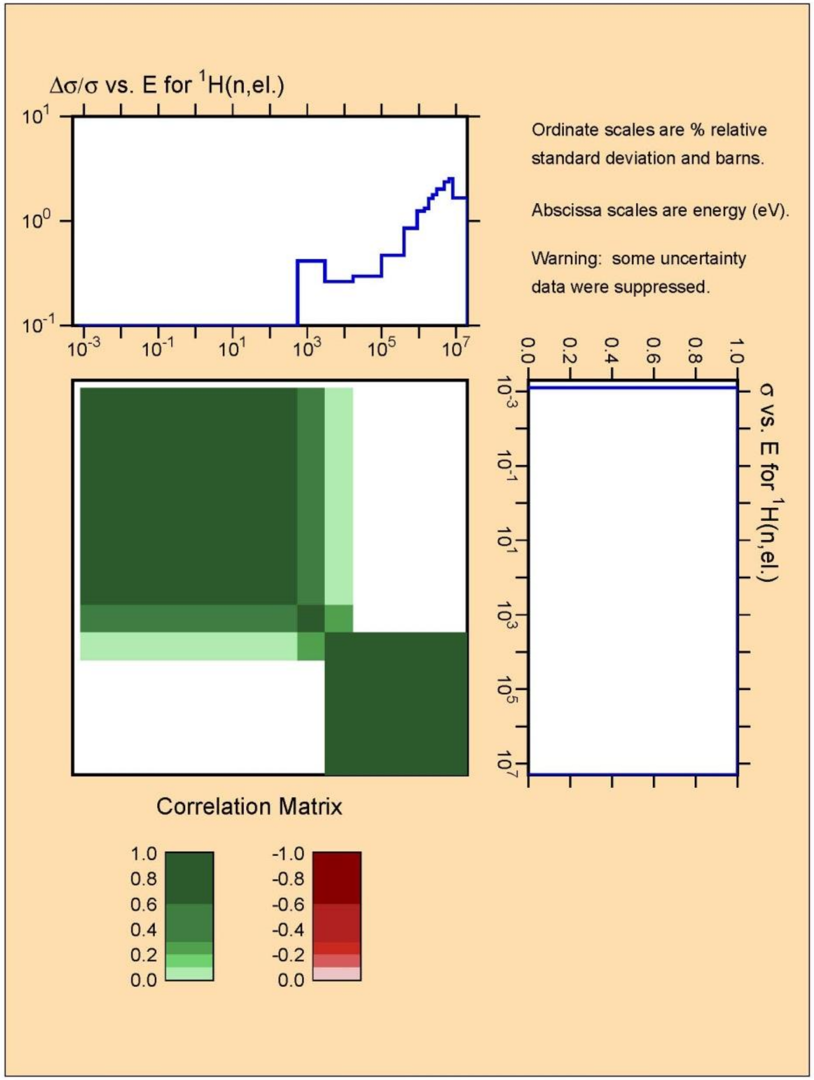


- **Comparison of relative standard deviation for different ENDFs sources**

- **Correlation matrix**



SCALE6.1 Correlation Matrix for Elastic Cross Section of Hydrogen (H)



Processing SCALE6.1/UN into ERRROR/BOXER format:

- ANGELO programme to convert COVERX into ERRORR
- LAMDA to check covariance properties
- NJOY, to process in BOXER format and to visualize with VIEWR

I.2 Methodology to generate random inelastic cross sections for H in H2O

The central (or nominal) values for all model parameters to be used in LEAPR are the values used for the JEFF-3.1.1 evaluation. In this work, seven different parameters were changed:

1. the translational weight ω_t (~ 25%)
2. the oscillator weights ω_j (~ 25%)
3. the free atom cross section for the scatter σ_1 (~10%)
4. the free atom cross section for the scatter σ_2 (~15%)
5. the frequency spectrum $\rho(\beta)$ (~30%)
6. the α value (~ 25%)
7. the β values (~ 25%)

Generating random files:

- Uniform PDFs were assumed
- Uncertainties of the above parameters were chosen in an ad-hoc way
- No information on how to choose the uncertainties of these parameters in the open literature
- Main constraint in the selection of these uncorrelated uncertainties was to reproduce the spread of the experimental inelastic cross section (as shown in Figure 1)
- Each of these parameters has a different influence on the inelastic cross section.
- Because of the high nonlinearity of $S(\alpha,\beta)$ equations, their combined effect is not equal to the linear sum of their independent effects.

I.3 Random Inelastic Cross-Section: H in H2O

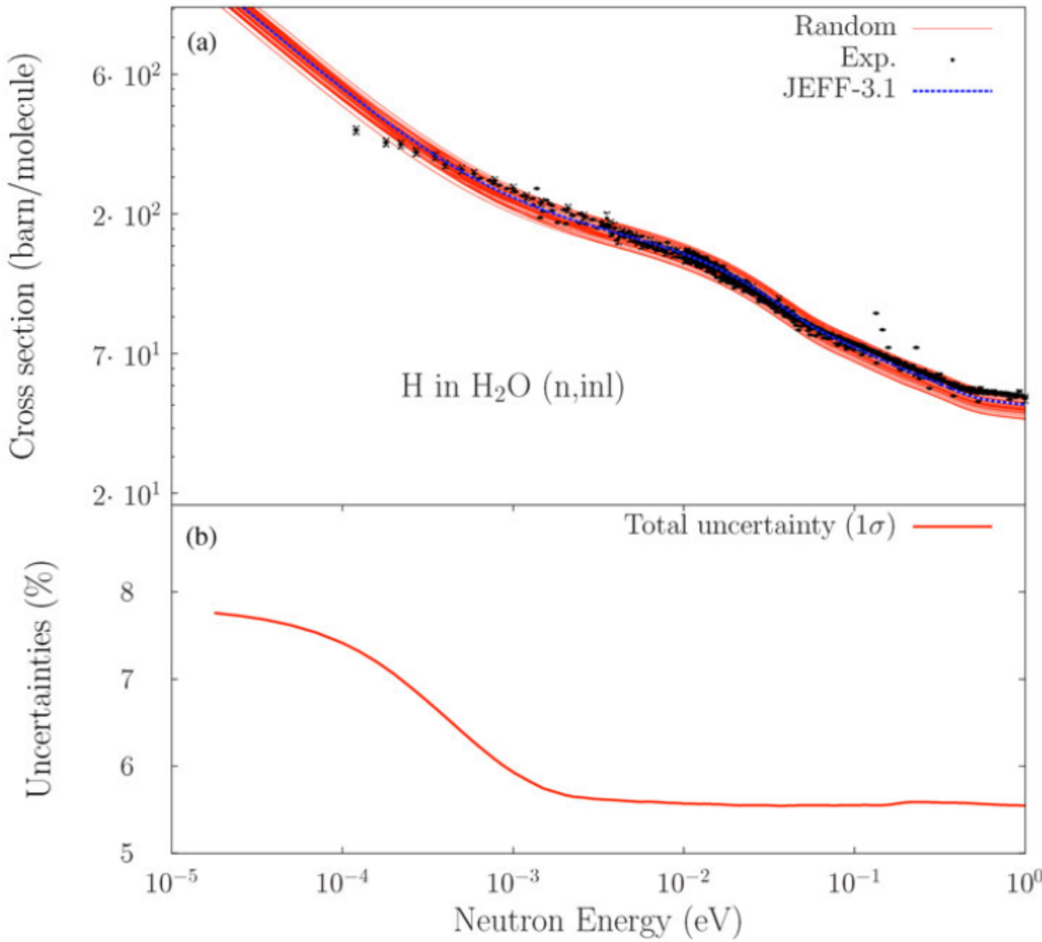


Figure 1. Incoherent random inelastic scattering cross section of H in H2O compared to experimental data and the inelastic cross section from the JEFF-3.1 library

Figure 2. Uncertainties in the inelastic cross section calculated from 1330 random inelastic cross sections

I.4 Correlation Matrix for Inelastic Cross Section: H in H2O

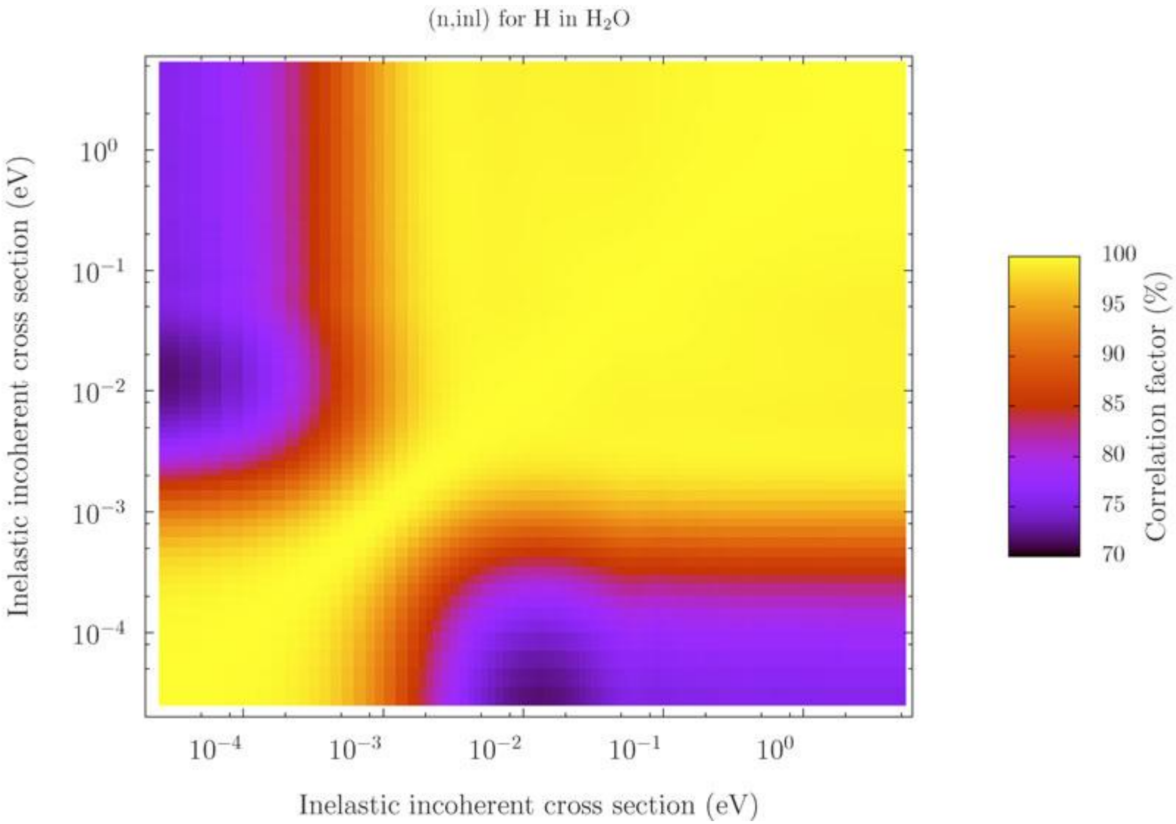


Figure 3. Energy-energy correlation matrix for the incoherent inelastic scattering of H in H2O. Note that the correlation values are always larger than 0.7.

I.5 Thermal Scattering Processed Data

In the specific case of the thermal scattering data for H in H2O, the procedure varies from the previous applications of the Petten adjustment method, but the philosophy stays the same. In order to generate thermal scattering data that can be used in a simulation, the following steps were taken:

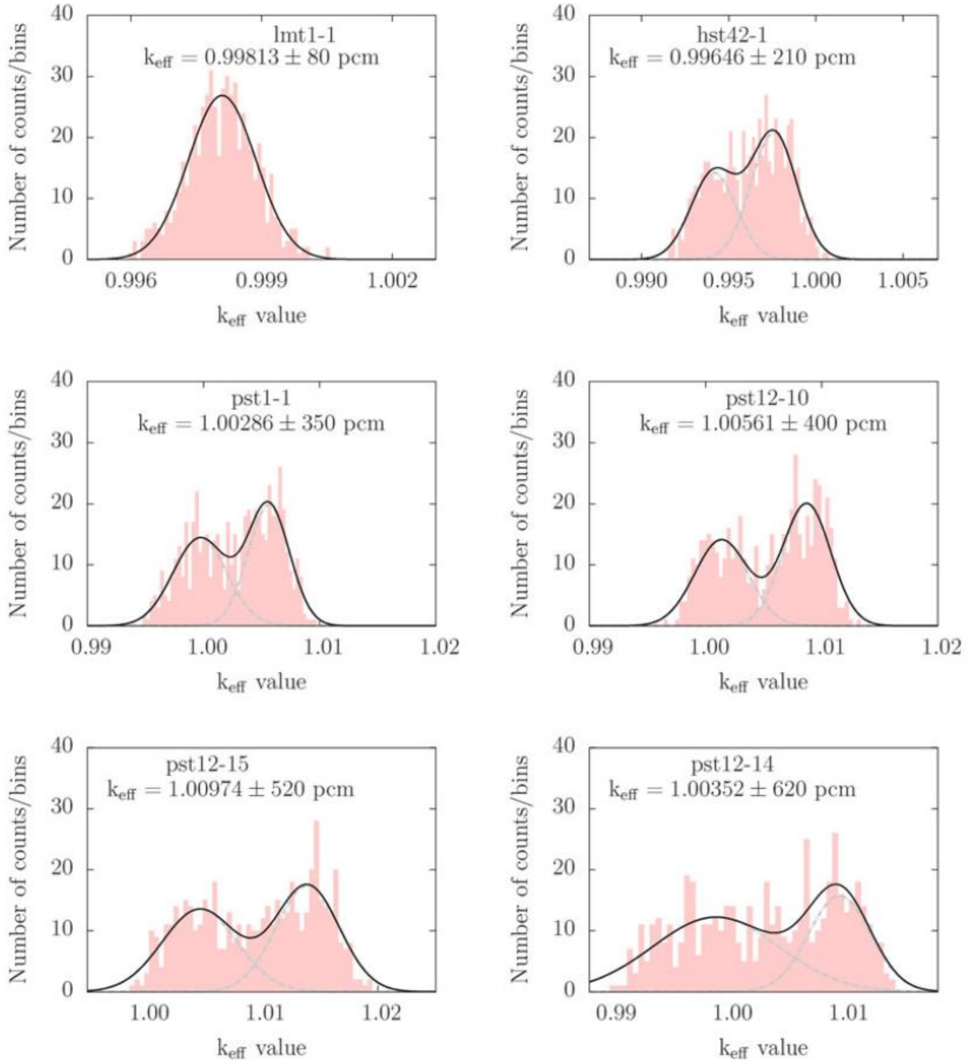
1. Create input parameters for the LEAPR (module of NJOY)
2. Run LEAPR to generate thermal scattering data in ENDF format “MF 7, MT 4” [incoherent inelastic data in terms of $S(\alpha,\beta)$ tables for different temperatures]
3. Use the ENDF file with the THERMR module of NJOY to generate pointwise thermal scattering cross sections.
4. Use the ENDF file and the output of THERMR with the ACER module of NJOY to generate thermal scattering data for the MCNP code in the ACE format.
5. Finally, repeat *n* times the previous steps with random input parameters for LEAPR.

I.6 Application to Criticality Benchmarks moderated by H2O

Figure 4. Calculated *keff* values for six benchmarks. Note that the total standard deviation is increasing from the top left figure to the right bottom figure.

The fits by one or two Gaussians are not used to extract the standard deviations but are presented to emphasize potential shifts from a Normal distribution.

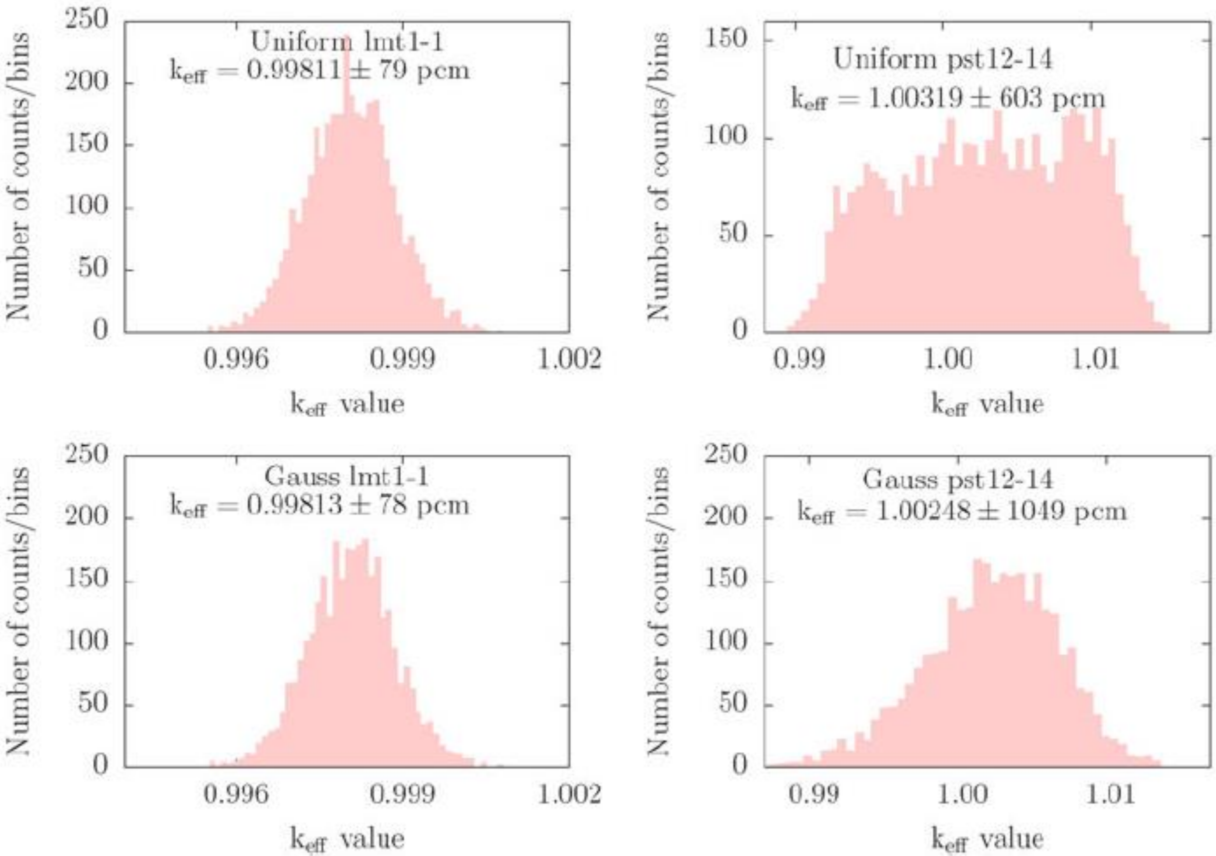
It is interesting to notice that the benchmarks with the higher sensitivity to the H in H2O thermal scattering data are the plutonium benchmarks (denominated “pst”) and not the uranium benchmarks (“lmt”).



I.7 Analysis of the Importance of PDF

Figure 5. Calculated *keff* values for two benchmarks: pst12-14 and lmt1-1 for two different distributions of the random model parameters: uniform (top plots) and Normal (bottom plots).

So, the non-Normal distributions in Figure 4 can be attributed to the uniform distributions for the model parameters.



PART II. SEANAP System

Ref. "*Continuous Validation and Development for Extended Applications of the SEANAP Integrated 3D PWR Core Analysis System*", C. Ahnert, J.M. Aragonés, O. Cabellos & N. García-Herranz, M&C99 (1999)

II.1 Introduction to SEANAP

SEANAP = Sistema Español de Análisis de Núcleos de Agua a Presión

SEANAP system has been developed and applied for 3D PWR core analysis during near thirty years, as a close collaboration among the Polytechnical University of Madrid group of developers (J. M. Aragonés et al.) and the engineering groups of users at the several Spanish PWR units.

SEANAP is a mature, demonstrated, complete and integrated system of computer codes and procedures that provide full and independent PWR core analysis capabilities.

- **Integrated /coupled codes in SEANAP:**

  MARPIJ, COBAYA, DELFOS, SIMULA, SIMTRAN, COBRA, RELAP-5

- **SEANAP Applications:**
  - *Fuel Loading Pattern Evaluations*
  - *Nuclear Design Analysis*
  - *On line 3D Simulations*
  - *Planning of Optimal Operational Maneuvers*
  - *Dynamic Core Analysis for Safety and Training Simulations*

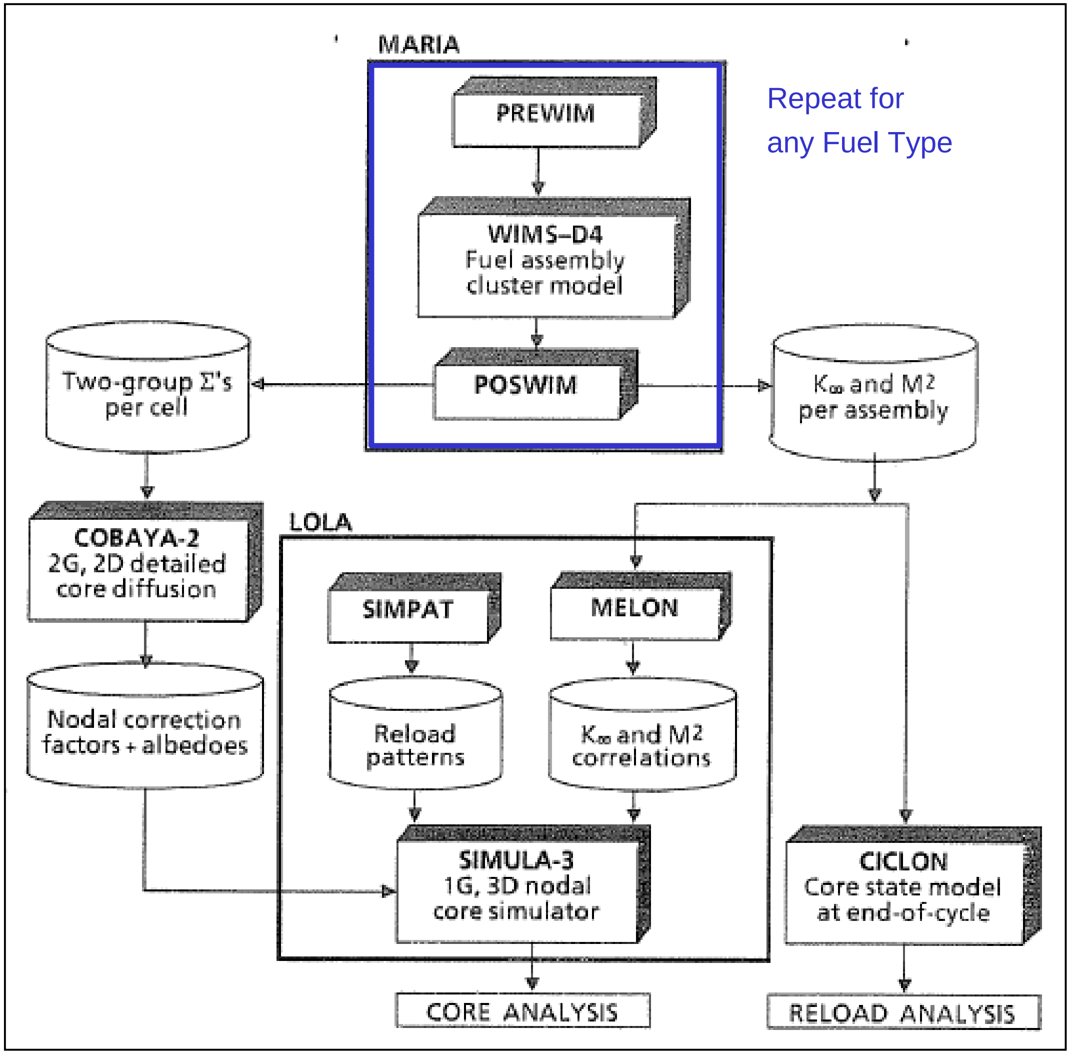
II.2 Scheme of the PWR Core Analysis SEANAP System

Figure 6. Scheme of the PWR Core Analysis System SEANAP-86

[*Ref. "Validation of PWR Core Analysis system SEANAP-86 with measurements in test and operation", C. Ahnert et al., M&C87*]

SEANAP is integrated by 4 subsystems:

1. **MARIA** system for assembly calculations
2. **COBAYA** system for a detailed (pin-by-pin) core calculations at reference conditions
3. **SIMULA** system for 3D 1 group corrected-nodal core simulation
4. **CICLON** system for fuel management analysis of reload cycles



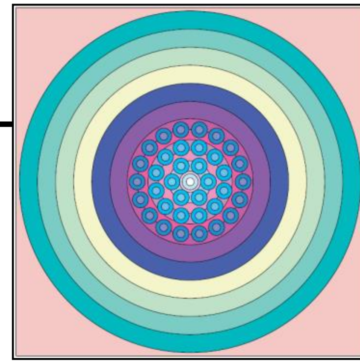
II.3 Scheme of the Cross-Section Generation for SEANAP System

Figure 7. Scheme of the PWR Core Analysis System SEANAP

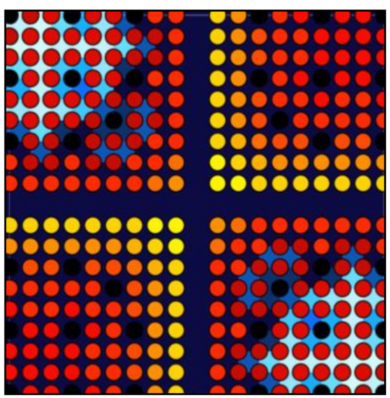
WIMSD-1986
69 GROUPS
(WIMS-R)

WIMSD-MARÍA
PWR fuel assembly calculations in 24 groups by S6 transport, in annular cluster geometry

Energy collapsing and spatial homogenization

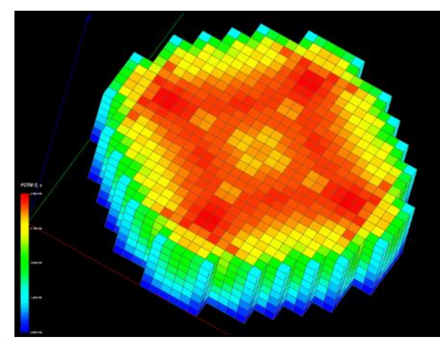


COBAYA
Pin-by-pin 2D calculations of full core planes, including radial reflector with a finite difference 2 group diffusion calculation



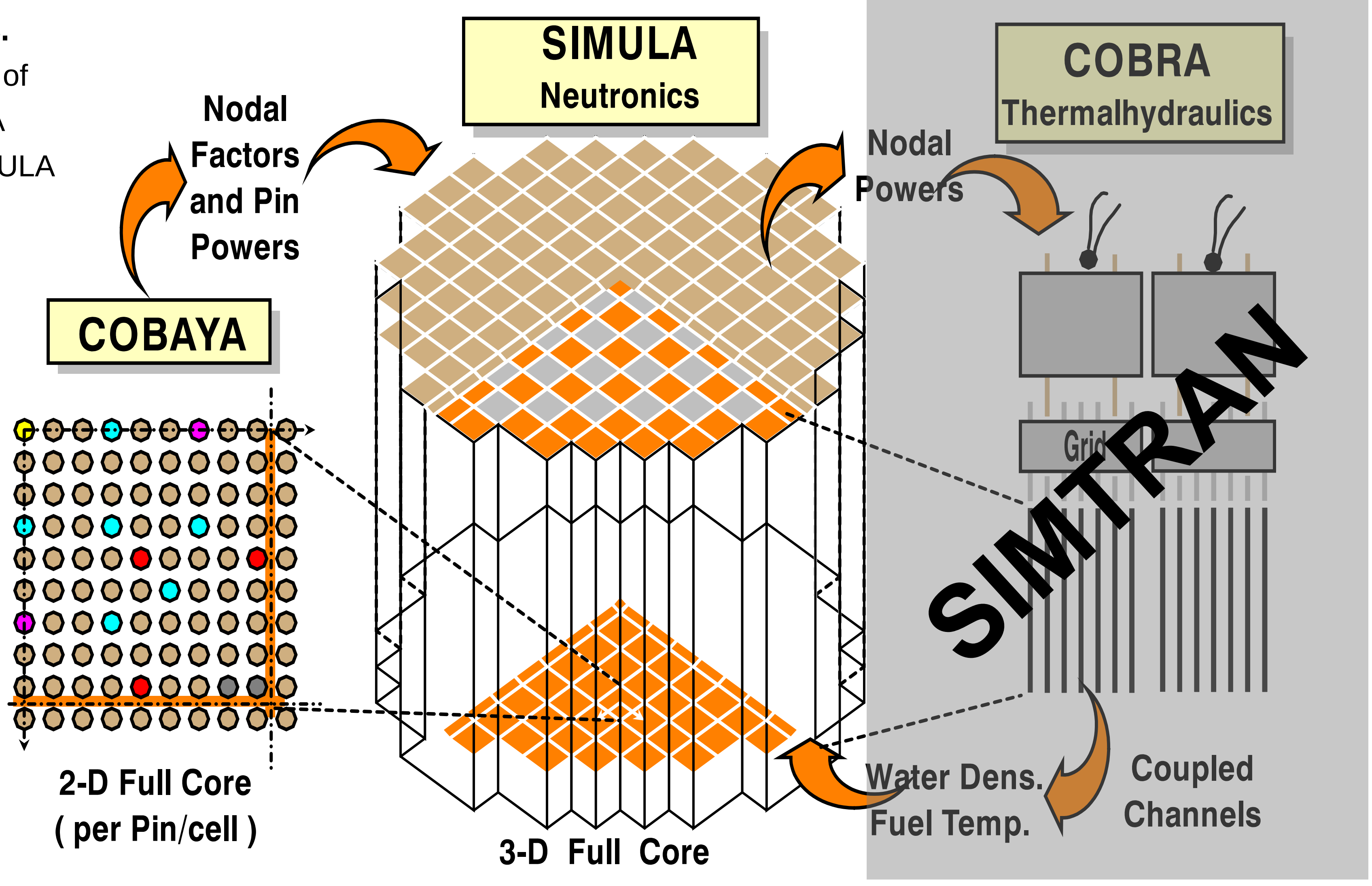
Energy collapsing and spatial homogenization

SIMULA
Nodal (1/4 assembly) 3D
Linear-discontinuous finite-difference coarse-mesh 1group diffusion with simplified close-channel subcooled-water thermalhydarulics



II.4 COBAYA and SIMULA

Figure 8. Scheme of COBAYA and SIMULA coupling



II.5 Validation of SEANAP

- SEANAP system has been applied in the last 30 years for 7 Spanish PWR units (Almaraz I and II, Ascó I and II, Trillo, Vandellós II and Zorita):
  - Fuel loading pattern optimization carried out for about **75 cycles** with very positive results
  - Full capability of the nuclear design for each cycle
    - **Start-up physic test at HZP**: critical end-point boron concentration , isothermal temperature coefficients, control bank worths, differential boron worth and power distribution
    - **Nominal operation**: boron concentration, in-core flux maps

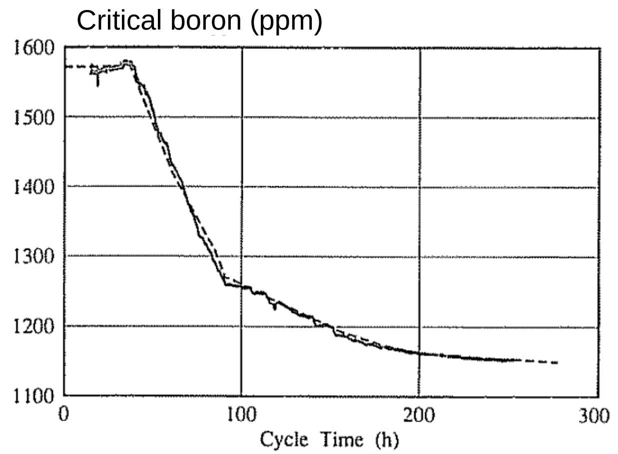


Figure 9. Critical boron (ppm) as a function of time (hours) from startup of cycle 8 in VandellosII: predictions (solid line) and chemical measurements (dashed line)

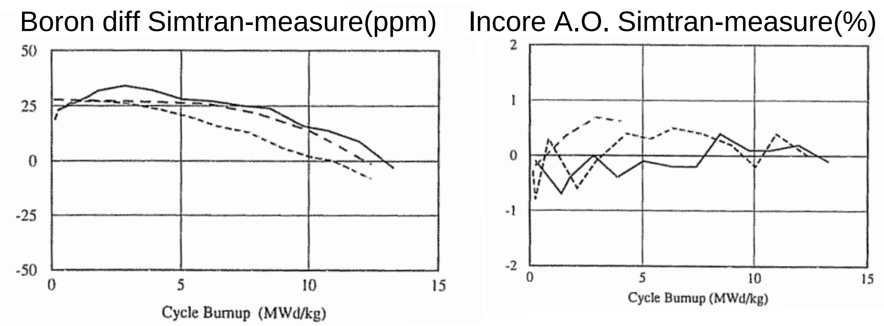


Figure 10. Diffreences Calculated_Measured in critical boron (ppm) and in-core axial offset (%) as a function of core burnup along cylces 6(dashed-line), 7 (solid line) and 8 (long dashed line) of Vandellos-II

II.5 Validation of SEANAP

- SEANAP system has been developed and implemented as an online simulator ~**20 cycles of three PWRs (Vandellós-II, Ascó-I and Ascó-II)**
  - **Every 5 minutes, continuos operational surveillance:** boron concentration, reaction rates at the excore detectors, A.O., fluid temperatures at the location of thermocouples, temperatures at the hot legs…
  - **Every month** incore flux maps: Incore/excore calibrations
  - **Planning of Optimal Maneuvers**, **Dynamic Core Analysis** for safety and training for plant engineers and operators.

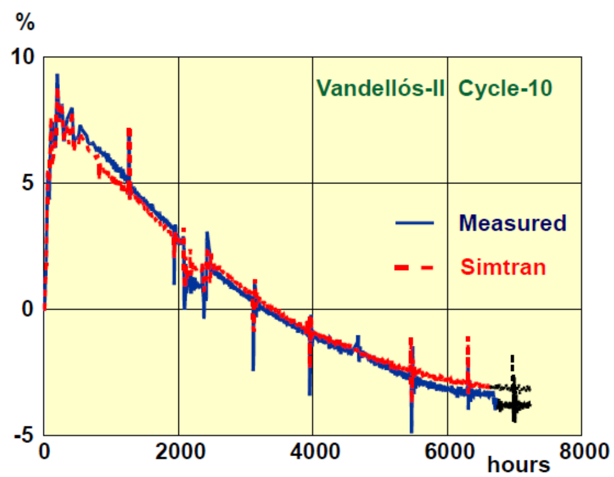


Figure 11. Delta-I of Incore Power as Measured and Calculated by SIMTRAN on-line

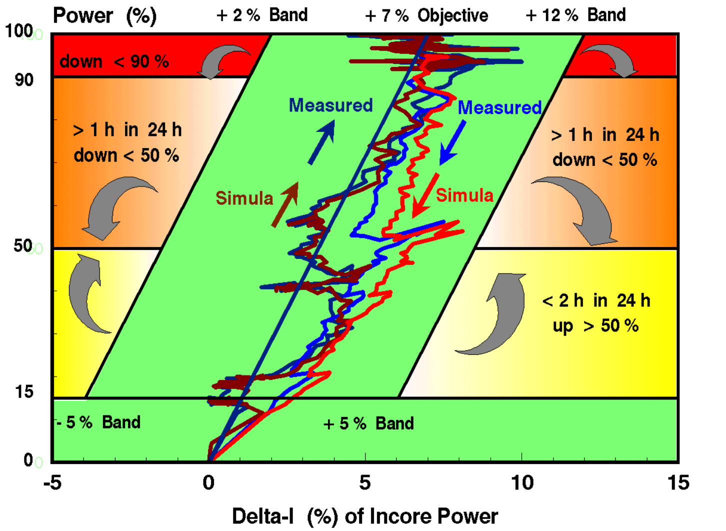


Figure 12. Measured and Simulated Power vs Delta-I in return to Power after a Short Shutdown

PART III. STLs Uncertainty Propagation in a PWR

- III.1 Random STL processing with SEANAP System
- III.2 PWR Core Analysis
- III.3 Uncertainty Quantification

III.1 Random STL processing with SEANAP System

Random STL/ENDF

NJOY/WIMSR processing

WLUP/willie program for updating WIMSD library

Repeat ~700 **histories**

CPU time:

~700* 8 min

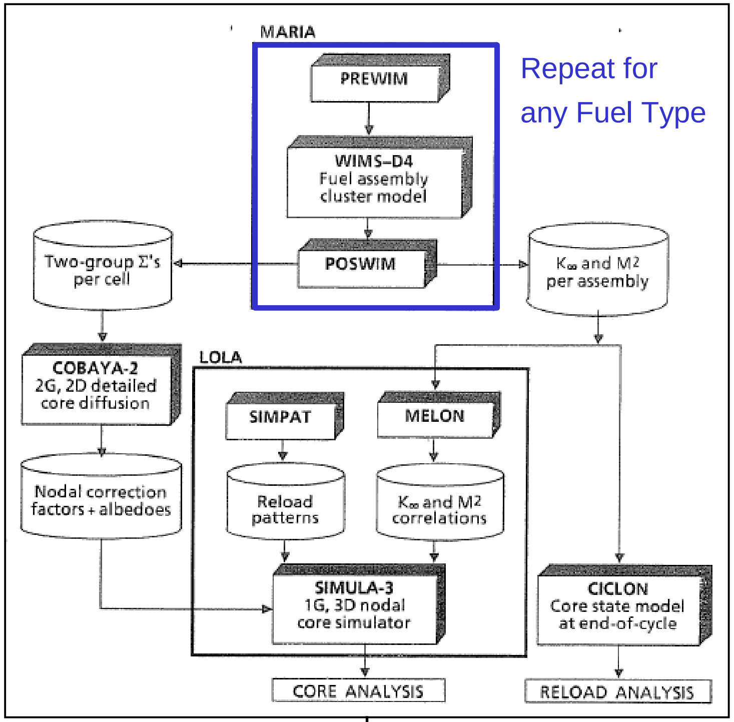


Figure 13. Scheme of TMC for random STL analysis

III.2 PWR problem description

PWR (WESTINGHOUSE), 3 loops , 157 FA, power 2775. MWth

¼ CORE

	1	2	3	4	5	6	7	8
1	1	13	4	**21**	6	**21**	16	14
2	13	11	15	2	16	6	**20**	7
3	4	15	3	**21**	8	**22**	**19**	
4	**21**	2	**21**	9	18	**20**	5	
5	6	16	8	18	12	17		
6	**21**	6	**22**	**20**	17			
7	16	**20**	**19**	10				
8	14	7						

AVE. BURNUP PER FUEL ASSEMBLY

	1	2	3	4	5	6	7	8
1	18.137	11.662	27.397	**0.000**	30.867	**0.000**	14.984	11.662
2	11.662	16.188	13.130	28.902	12.155	28.866	**0.000**	30.191
3	27.397	13.130	27.572	**0.000**	22.778	**0.000**	**0.000**	
4	**0.000**	28.902	**0.000**	30.755	15.236	**0.000**	30.124	
5	30.867	12.155	22.778	15.236	13.123	14.882		
6	**0.000**	28.866	**0.000**	**0.000**	14.882			
7	14.984	**0.000**	**0.000**	30.503				
8	11.662	30.191						

FUEL	TYPE	w/o(%)	WABAS
1	OFA	2.10	0
2	OFA	3.10	0
3	OFA	3.24	0
4	OFA	3.24	0
5	OFA	3.24	0
6	OFA	3.24	0
7	OFA	3.24	0
8	OFA	3.24	0
9	OFA	3.24	0
10	OFA	3.24	0
11	OFA	3.24	0
12	AEF	3.60	0
13	AEF	3.60	0
14	AEF	3.60	0
15	AEF	3.60	0
16	AEF	3.60	0
17	AEF	3.60	0
18	AEF	3.60	0
19	AEF	3.60	0
20	AEF	3.60	4
21	AEF	3.60	8
22	AEF	3.60	12

III.3 Uncertainty Quantification

Burnup (GWd/TMU)	Boron (ppm)	1 σ	A.O. (%)	1 σ	Fz	1 σ	FΔH	1 σ	FQ	1 σ
0.0 HZP	1558	21	28.7	0.6	1.539	0.003	1.578	0.005	2.444	0.013
0.0 HFP	1374	24	6.2	1.0	1.289	0.001	1.469	0.003	1.912	0.002
0.2	1034	24	0.9	0.7	1.234	0.003	1.426	0.003	1.788	0.003
0.5	992	24	0.1	0.6	1.215	0.003	1.420	0.002	1.757	0.004
1.0	941	23	-0.5	0.5	1.199	0.004	1.423	0.003	1.744	0.003
2.0	848	22	-1.6	0.3	1.170	0.004	1.428	0.003	1.716	0.003
3.0	754	22	-2.3	0.2	1.147	0.003	1.427	0.003	1.689	0.001
4.0	659	21	-2.9	0.1	1.133	0.002	1.422	0.003	1.667	0.002
5.0	563	21	-3.1	0.0	1.125	0.001	1.416	0.003	1.649	0.002
6.0	469	21	-3.3	0.0	1.122	0.001	1.409	0.002	1.638	0.002
7.0	375	20	-3.4	0.0	1.121	0.000	1.404	0.002	1.633	0.003
8.0	283	20	-3.4	0.0	1.118	0.000	1.400	0.002	1.625	0.003
9.0	192	20	-3.1	0.0	1.113	0.000	1.396	0.001	1.610	0.002
10.0	103	19	-2.8	0.0	1.109	0.000	1.393	0.001	1.596	0.002
11.0	16	19	-2.8	0.0	1.107	0.000	1.390	0.001	1.588	0.002
12.0	-70	19	-2.8	0.0	1.108	0.001	1.386	0.001	1.577	0.002

III.3 Uncertainty Quantification

Burnup (GWd/TMU)	Vboro (pcm/ppm)	1 σ	CTM (pcm/C)	1 σ	CTISO (pcm/C)	1 σ	CPDop (pcm/%)	1 σ	CPOT (pcm/%)	1 σ
0.0 HZP	-8.25	0.01	-3.5	0.9	-8.7	0.9	-16.27	0.02	-21.1	0.2
0.0 HFP	-7.83	0.01	-22.6	1.2	-26.0	1.2	-10.45	0.02	-19.4	0.2
0.2	-7.88	0.01	-31.0	1.2	-34.4	1.2	-10.54	0.03	-20.8	0.3
0.5	-7.89	0.00	-32.3	1.2	-35.7	1.2	-10.47	0.03	-20.9	0.3
1.0	-7.90	0.00	-34.1	1.2	-37.4	1.2	-10.41	0.03	-21.2	0.3
2.0	-7.94	0.01	-37.2	1.1	-40.6	1.1	-10.27	0.04	-21.8	0.3
3.0	-8.00	0.01	-40.3	1.1	-43.7	1.1	-10.16	0.04	-22.4	0.3
4.0	-8.09	0.01	-43.3	1.1	-46.6	1.1	-10.08	0.04	-22.9	0.3
5.0	-8.20	0.02	-46.2	1.0	-49.5	1.0	-10.03	0.04	-23.4	0.3
6.0	-8.31	0.02	-49.1	1.0	-52.4	1.0	-10.02	0.04	-24.0	0.3
7.0	-8.44	0.02	-51.8	1.0	-55.2	1.0	-10.04	0.04	-24.6	0.3
8.0	-8.57	0.02	-54.6	1.0	-57.9	1.0	-10.09	0.05	-25.2	0.3
9.0	-8.70	0.02	-57.3	0.9	-60.6	1.0	-10.15	0.05	-25.8	0.2
10.0	-8.84	0.03	-59.9	0.9	-63.3	0.9	-10.23	0.05	-26.4	0.2
11.0	-8.98	0.03	-62.6	0.9	-66.0	0.9	-10.29	0.05	-27.0	0.2
12.0	-9.13	0.03	-65.1	0.9	-68.6	0.9	-10.33	0.05	-27.5	0.2

III.3 Uncertainty Quantification: PDFs

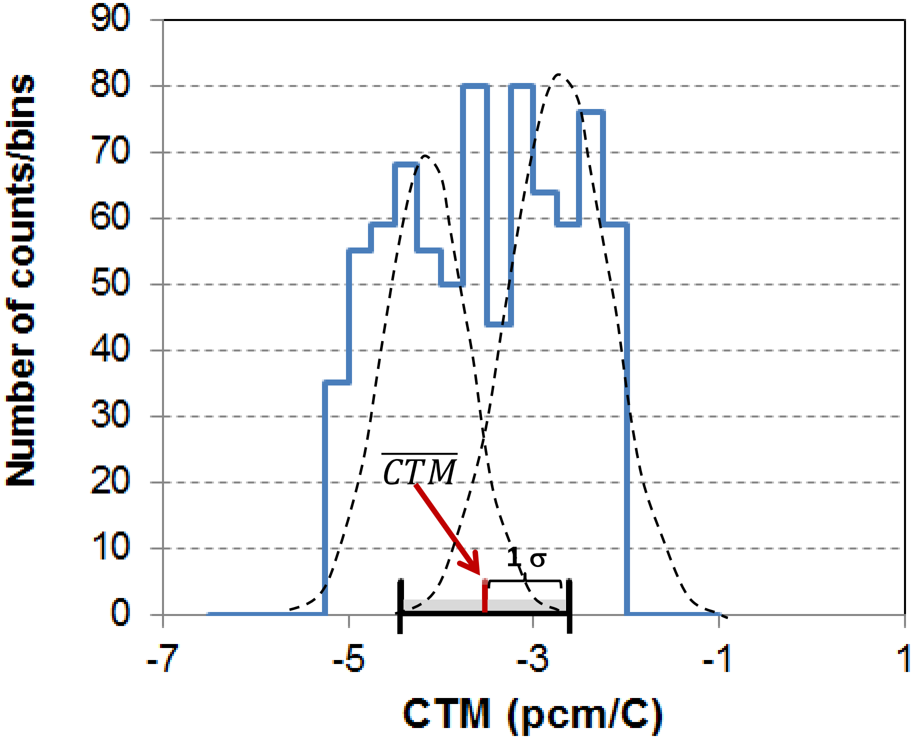


Figure 14. Calculated CTM(pcm/C) at BOC

Summary and conclusions

- Random STLs provided by NRG to be used in a PWR core analysis
- Application of SEANAP system in Uncertainty Analysis
- Uncertainty Quantification of PWR “*Nuclear Reactor Design*”

Acknowledgements

This work is partially supported by:

- *Agreement between CSN & UPM in the area of “Uncertainty Propagation for Neutronic Calculations” (2012-16)*
- *Fellowship “Cátedra Federico Goded “, CSN/Department of Nuclear Engineering (UPM)*
- *Fellowship“F2I2”, ETSII (UPM)*